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14. ABSTRACT

In this report, we summarize the research that has been accomplished under the sponsorship of the Army Research Office (W911NF-12-1-0023). Ab initio calculations have been performed to study the effects of solute atoms on the c/a ratio of magnesium alloys. Atomistic simulations have also been performed to investigate the interaction between a Mg17Al12 precipitate and a {10-12}<10-1-1> twin boundary. Interactions between a Mg17Al12 precipitate and the basal slip and the prismatic slip have been performed as well. In addition, experiments of

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Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

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Number of Manuscripts:

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Patents Awarded

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Names of Post Doctorates

NAME	PERCENT_SUPPORTED
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Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Mark Horstemeyer	0.10	
Bin Li	0.20	
FTE Equivalent:	**0.30**	
Total Number:	**2**	

Names of Under Graduate students supported

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Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

(1) Density Function Theory (DFT) calculations of the effects of alloying elements on the c/a ratio of magnesium were performed. The most commonly and extensively used alloying elements such as Al, Mn, and Zn were calculated. Other alloying elements such as In, Li and some rare earth elements Y, Ce were calculated as well. Generally, Al and Li decrease the c/a ratio and this trend is consistent with experimental observations. The DFT calculations also show that Zn decreases the c/a ratio as well, but experiment measurements show that solutionized Mg-Zn alloys present little change in the c/a ratio. Notably, the rare earth elements significantly increase the c/a ratio. These elements have been added to Mg alloys to randomize the texture. Increase in the c/a ratio will decrease deformation twinning and randomize the texture.
The effects of the alloying elements on the c/a ratio also depend upon the actual state of the solute atoms. Zn tends to form short range ordering in Mg alloys. Hence, more calculations on the energetically favorable state of different configurations of solute atoms are needed.
(2) Interactions between Mg17Al12 precipitate and {10-12}<10-1-1> twin boundaries (TBs) in magnesium were studied by molecular dynamics simulations. The results obtained well agree with experimental observations in which precipitates can be entirely engulfed by {10-12}<10-1-1> twins without being sheared. Structural analysis of the TBs in the atomic scale shows that the TBs are extremely incoherent during twin growth and highly deviate from the {10-12} twinning plane, well consistent with experimental observations too. It was observed that {10-12}<10-1-1> twinning was accomplished solely by atomic shuffling that converts the parent lattice to the twin lattice without involving twinning dislocations at all, resulting in zero shear strain at the TBs. Consequently, the precipitate remained unsheared while the TBs were passing the precipitate. Our results demonstrate how and why the current Mg alloy design philosophy does not work.

Technology Transfer

W911NF-12-1-0023

REPORT

Toward New Magnesium Alloy Design - Theoretical and Experimental Studies of the Influence of Alloying Elements on Deformation Twinning

M.F. Horstemeyer

Center for Advanced Vehicular Systems (CAVS), Mississippi State University

Submitted to ARO

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List of Illustrations and Tables

Abstract

In this report, we summarize the research that has been accomplished under the sponsorship of the Army Research Office (W911NF-12-1-0023). *Ab initio* calculations have been performed to study the effects of solute atoms on the *c*/*a* ratio of magnesium alloys. Atomistic simulations have also been performed to investigate the interaction between a $Mg_{17}Al_{12}$ precipitate and a $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twin boundary. Interactions between a $Mg_{17}Al_{12}$ precipitate and the basal slip and the prismatic slip have been performed as well. In addition, experiments of deformation behavior of an AZ91 Mg alloy heat-treated under different conditions have been conducted. More calculations and simulations, and systematic experimental studies are needed to obtain conclusive data. Some of the results are summarized in this report.

1. Introduction

Unlike face-centered-cubic (fcc) metals, metals with hcp crystal structures, e.g., Mg, Ti, Zr, and Co, contain only limited number of easy slip systems that cannot accommodate plastic strain in the [0001] direction. For Mg in particular, the primary slip system is $(0001)<2\bar{1}\bar{1}0>$ with a magnitude 0.321 nm. When Mg alloys are loaded at all strain rates and over a whole range of temperatures of thermomechanical processing, profuse twinning is activated in the microstructure and rapidly reorients the crystals. The primary twinning system for all hcp metals is $\{10\bar{1}2\}<10\bar{1}\bar{1}>$. In classical twinning theories [1,2], the magnitude of the Burgers vector of the theoretical twinning dislocation for Mg is only 0.024 nm, which is a tiny fraction of any matrix dislocation in hcp metals. Such a small twinning Burgers vector gives rise to unique properties of this ubiquitous twinning mode in hcp metals:

(1) *Low critical stress*. The exceptionally small twinning Burgers vector (0.024 nm for Mg) implies that the twin lattice almost exists in the parent lattice before any twinning shear is applied, and only local adjustments by atomic shuffling are needed to accomplish twinning [3]. Though the critical stress of the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning was estimated higher than the basal slip [4], such estimation is questionable because precise measurement of the critical stresses of twinning and slip in hcp metals is difficult. In fact, some experiments have shown that the critical stress of the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning could be lower than that of the basal slip [5].

(2) *High twin volume fraction*. The volume fraction of deformation twins can reach as much as 80% or more when twinning is saturated. Parent grains can be twinned completely.

(3) *Extremely high mobility of twin boundaries*. Atomistic simulations [3] and experimental observations [5, 6] have shown that the actual twin boundaries can significantly deviate from the $\{10\bar{1}2\}$ twinning plane, suggesting that this twinning mode is indeed controlled by atomic shuffling. Even small stresses can cause the twin boundaries to migrate and evolve into extreme incoherency [5].

(4) *Profuse twinning at high temperatures*. Contrary to the belief that at elevated temperatures dislocation slip is dominant over twinning, our recent experiments show that, even at 450°C, and with compression at strain rates above 0.5/s, high density twins are still observed in a Mg alloy [7]. These strain rates are lower than those in conventional rolling and extrusion of Mg alloys, and higher strain rates favor twinning.

(5) *Reversible twinning and non-Schmid effect*. The $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning presents pseudoelasticity or reversible twinning [8,9]. When external stress is removed or reversed, twins can shrink or even disappear. Experiments also observed that this twinning mode may disobey the Schmid Law [10].

These properties drastically differ from fcc metals in which dislocation slip dominates plastic deformation. Another significant difference is that the generalized stacking fault energy [11] cannot properly describe the shuffling-dominated $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning. For twinning-dominated deformations, alloy design based on dislocation-impedance interactions has only achieved limited success [12]. To control the mechanical properties of hcp metals, we have to conduct fundamental research to understand how alloying elements influence deformation twinning in terms of twin volume fraction and twin boundary mobility, and interactions between twinning and slip, and interactions between precipitates and twins.

With the support of the ARO, we have conducted *ab initio* calculations of the effects of alloying elements on the *c*/*a* ratio which is an important structural parameter for deformation twinning; interactions between a $Mg_{17}Al_{12}$ precipitate and a $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twin boundary; and interactions between a $Mg_{17}Al_{12}$ precipitate and the basal slip and the prismatic slip. We also performed experimental studies on the deformation behavior of an AZ91 Mg alloy under different heat-treating conditions.

2. Methodology

All the DFT (density function theory) calculations were carried out with the Vienna Ab initio Simulation Package (VASP) [13] using the projector-augmented wave (PAW) basis set [14] and spin-dependent Perdew-Burke-Ernzerhof (PBE) [15-17] generalized gradient approximation (GGA) exchange-correlation functional. The unit cell size was 6×6×3, and the total number of the atoms in the calculation was 215. Periodic boundary condition was applied to all three dimensions.

In our molecular dynamics simulations, the interatomic potentials for Mg-Al binary alloys developed by Liu et al. [18] were used. The potentials are embedded atom method (EAM) type [19-20]. Data from force matching method were incorporated to improve the accuracy of the potentials. The potentials were fitted not only to the experimental data, but also to forces data obtained from *ab initio* calculations using local orbital pseudopotential based on the local density approximation in the density functional theory. Data from different structures, including bulk, cluster, liquid and defects, were included in their fitting. These potentials have been validated by extensive simulations and experiments of deformation behavior of Mg [21-22]. we simulated

pyramidal dislocations and the resultant stacking faults in Mg [21], zonal twinning dislocations that mediate $\{10\bar{1}1\}<10\bar{1}\bar{2}>$ twinning [7], and the mechanism for $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning [8]. These results obtained in our simulations are in good agreement with experimental observations [22]. The Liu's potentials satisfactorily describe twinning behavior in Mg and provide a stable structure of the β intermetallic phase ($Mg_{17}Al_{12}$). For this reason, we used the Liu's potentials in the present work to investigate interactions between a $Mg_{17}Al_{12}$ precipitate and $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twin boundaries.

Figure 1 shows the cross-section view of the initial configuration in which a Mg single crystal with a β-$Mg_{17}Al_{12}$ precipitate was constructed. For simplicity of analysis of the simulation data, we neglected the effect of alloying element (Al) on the motion of a TB and just used pure Mg rather than a Mg-Al solid solution to simulate the interaction between a TB and a $Mg_{17}Al_{12}$ precipitate. We only show a thin slice (~1.5 nm thick) of the system in the middle of through thickness direction. The basal planes of the matrix are perpendicular to the figure plane, and are colored in yellow and blue to show the *ABABAB*… hcp stacking from left to right. This color scheme in 2-D view was kept unchanged throughout the simulation such that the evolution in microstructure during deformation can be recognized with clarity. The system contains over one million atoms, with dimensions 40×20×20 nm^3. The crystallographic orientation of the Mg matrix is indicated in Figure 1. The $Mg_{17}Al_{12}$ precipitate has dimensions 10×10×10 nm^3, with a bcc structure and located in the center of the Mg matrix. The precipitate is colored differently from the matrix such that it can be readily identified during deformation. The matrix and the precipitate satisfy the predominant Burgers orientation relationship: $(0001)_M \parallel (011)_P$, and $[2\bar{1}\bar{1}0]_M \parallel [\bar{1}11]_P$. Although other orientation relationships were also reported [23-25], only the Burgers orientation relationship was considered in this work.

In our simulations, no pre-existing twin boundaries (TBs) were introduced into the system before the simulations started. The simulation scheme is such that twin nucleation and growth is initiated by an external strain. To obtain an extension twin, a tensile strain was applied by moving the atoms on the right-side end at a constant displacement rate of a/10,000 per time step (3.0 fs) along the [0002] direction, where a = 0.32094 nm is the lattice constant of Mg, corresponding to a strain rate about 8.0×10^8 s^{-1}. In this scenario, the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ extension twinning is favored. The resolved shear stresses on the basal plane and the prismatic plane are zero, so only pyramidal slip can be activated. The simulation temperature was kept constant at 10 K. Free surfaces were applied to all three dimensions.

2-D and 3-D plots were made to reveal the migration of the TB and the interaction between the TB and the precipitate. These plots are necessary to obtain unambiguous interpretation of the simulation results.

3. Results and discussions

3.1 Effects of alloying elements on the *c*/*a* ratio

First, we calculated the lattice parameters of pure Mg. Table 1 shows the *ab initio* results of the lattice parameters of pure Mg. Compared to the experimental measurements at room temperature, the calculated lattice parameters are slightly smaller than the experimental measurements at room temperature.

The effects of alloying elements on the *c*/*a* ratio of Mg from the *ab initio* calculations are summarized in Table 2. The most commonly and extensively used alloying elements such as Al, Mn, and Zn were calculated. Other alloying elements such as In, Li and some rare earth elements Y, Ce were calculated as well. Generally, Al and Li decrease the *c*/*a* ratio and this trend is consistent with experimental observations [26]. The *ab initio* calculations also show that Zn decreases the c/a ratio as well, but experiment measurements show that solutionized Mg-Zn alloys present little change in the *c*/*a* ratio. Notably, the rare earth elements significantly increase the *c*/*a* ratio. These rare earth elements have been added to Mg alloys to randomize the texture. Increase in the c/a ratio will decrease deformation twinning. It is well known that texture is closely related to deformation twinning which abruptly and efficiently change the orientation of the lattices in individual grains.

The effects of the alloying elements on the c/a ratio also depend upon the actual state of the solute atoms. Zn tends to form short range ordering in Mg alloys [27]. Hence, more calculations on the energetically favorable state of different configurations of solute atoms are needed.

The *ab initio* calculations provide valuable insights on this important issue that has significance in design and processing of Mg alloys. More *ab initio* calculations are needed to further understand how alloying elements affect the *c*/*a* ratio and hence the twinning behavior of Mg alloys.

3.2 Atomistic simulations of interactions between a precipitate and twinning

During straining along the [0002] direction, multiple pyramidal dislocations were produced. The 2-D and 3-D views of the pyramidal dislocations and the resultant stacking faults were shown in Figure 2a. These dislocations are on $\{10\bar{1}1\}$. It was shown that $\{10\bar{1}1\}<10\bar{1}\bar{2}>$ pyramidal slip is energetically more favorable than $\{11\bar{2}2\}<11\bar{2}\bar{3}>$ for hcp metals because its Burgers vector is smaller and the interplanar spacing is larger [21].

As the tensile strain increases, deformation twinning starts to take place. A $\{10\bar{1}2\}$ twin nucleated near the pyramidal dislocations. The twinned region is enclosed by the stacking faults and an incoherent TB delineated by the dashed pink line in Figure 2a can be observed. The TB does not match the $\{10\bar{1}2\}$ twinning plane. Notably it can be observed that, in the 2-D view, the TB appears hugely deviating from the $\{10\bar{1}2\}$ twinning plane. Such a deviation can be appreciated from the fact that part of the TB is nearly parallel to the basal plane of the matrix, whereas the theoretical twinning plane $\{10\bar{1}2\}$ should be at 43.1° with the basal plane. To better reveal the orientation relationship between the twin and the matrix, a circled area in Figure 2a that comprises both the matrix and the twin was magnified and shown in Figure 2b. In the

twinned region (bounded by the pink dashed line), the stacking of the basal planes was marked with capital letters *ABAB*… from bottom to top, whereas the stacking of the basal planes of the matrix was also marked with *ABAB*… but from left to right. Clearly, the basal plane of the matrix was reoriented by nearly 90°, typical of $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ extension twinning. An important observation is that, after twinning, the originally flat basal planes, i.e., the blue and yellow columns of atoms, convert to the corrugated prism planes of the twin, but the atoms remain nearly in the original vertical direction. In other words, the basal plane of the matrix did not experience a shear. To reveal this interesting phenomenon, we drew a vertical red line that crosses the atoms of a basal plane in the matrix and extends into the twin. In the twinned region, the yellow atoms reside on a double-layered prism plane which is geometrically not a flat plane, but on average, the double-layered prism plane nearly parallels to the matrix basal plane. Such a pattern unequivocally demonstrates that no shear strain was produced by the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning. 3-D view of the motion of the TB was plotted in Figure 2c. The TB is extremely incoherent in 3-D and does not coincide with a strictly defined crystallographic plane. In Figure 2c, part of the TB (indicated by the block arrow) is passing the precipitate. As the strain increases, the TB expands, and the precipitate is being engulfed while the matrix material in the front is being twinned. Meanwhile, more stacking faults were generated in the matrix.

As the tensile strain further increases, the twinned region continues to expand and reaches the surfaces, as shown in Figure 3, which is the final stage when the precipitate was engulfed by the twin. In the 2-D view, at the top and the bottom interfaces between the precipitate and the matrix, a thin layer of retaining matrix material can be seen, although the precipitate is entirely embedded inside the twin. In 3-D, the TB has swept over the precipitate without causing shear deformation to it. Some of the defects generated during deformation in the matrix prior to twinning were "cleaned" up by twinning.

Our simulation results confirm that a $Mg_{17}Al_{12}$ precipitate can indeed be engulfed by $\{10\bar{1}2\}$ deformation twins without being sheared while the TB is passing the precipitate. Our simulations also reveal that the TBs are extremely incoherent and can hugely deviate from the $\{10\bar{1}2\}$ twinning plane. In other words, the twinning plane of this predominant twinning mode for hcp metals is far from strictly defined. This phenomenon vastly differs from other twinning modes in hcp, fcc and bcc metals in which a twin boundary has to match the twinning plane at least in the atomic scale, although microscopically small deviations no more than a few degrees are allowed due to the presence of twinning dislocation loops at the TB and strain accommodation. It is required that a TB match the twinning plane because a twinning plane has to be an "invariant plane" during straining [2] and the glide of twinning dislocations is strictly confined in the twinning plane. If $\{10\bar{1}2\}<10\bar{1}\bar{2}>$ twinning were mediated by twinning dislocations, as suggested previously [28-29], we would expect a strong interaction between the precipitate and the twinning dislocations. The twinning dislocations would either shear the precipitate if $Mg_{17}Al_{12}$ is deformable, or be impeded at the precipitate/matrix interface if $Mg_{17}Al_{12}$ is non-deformable. Either of these two cases would result in strengthening to the material, especially if the

intermetallic precipitate is non-deformable. But these interactions did not occur in experiments [30,31] and in our atomistic simulations.

The experimental observations and our simulations strongly suggest that $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning in hcp metals is not mediated by twinning dislocations. In fact, if $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning were controlled by twinning dislocations, the extensively observed reversible twinning in Mg [8-9] should not happen because dislocation-dominated plastic deformation in crystalline materials is irreversible.

It was demonstrated [3] that atomic shuffling is all needed to accomplish the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning, without involving well-defined twinning dislocations. In this model [3], the lattice conversion between the twin and the parent is achieved by atomic shuffling that converts the parent basal planes to the twin prism planes, and the parent prism planes to the twin basal planes. This direct lattice conversion requires atomic shuffling to create correct hcp lattice and twin orientation relationship. No twinning shear is involved at all. Because of the shuffling dominated twinning, the twin boundaries can pass precipitates, but leaving the precipitates unsheared. Also, because no twinning dislocations are involved, the actual twin boundaries do not have to match the $\{10\bar{1}2\}$ twinning plane and can be extremely incoherent, as seen in our simulations.

4. Concluding remarks

Under the sponsorship of the ARO (W911NF-12-1-0023), *ab initio* calculations have been conducted to study the effect of alloying elements on the *c*/*a* ratio of Mg alloys which is an important structural parameter in deformation twinning. The results show that Al and Li decrease the *c*/*a* ratio and hence enhance deformation twinning, but the rare earth elements such as Y and Ce increase the *c*/*a* ratio.

Atomistic simulations have been performed as well to investigate the interactions between a $Mg_{17}Al_{12}$ precipitate and deformation twinning. The results show that the precipitate can be engulfed by a moving twin boundary without being sheared. These results are consistent with experimental observations.

The simulations results obtained in this research are promising and can be used as guidelines for design of new Mg alloys to achieve optimized mechanical properties. Further studies including cross-scale calculations and simulations and experiments are needed for a more systematic investigation.

5. Publications and presentations

A number of journal publications and conference presentations are being prepared and will be submitted to the leading journals of materials science and engineering.

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Table 1. *Ab initio* calculations of the lattice parameters of pure Mg

	a	*c*
Ab initio	3.2035	5.14567
Experiment (300 K)	3.2094	5.21

Table 2. *Ab initio* calculations of effects of alloying elements on c/a ratio

Solute	Δ(c/a)
Al	-0.095
Li	-0.098
Zn	-0.314
Mn	-0.204
In	-0.039
Ce	0.309
Y	0.153

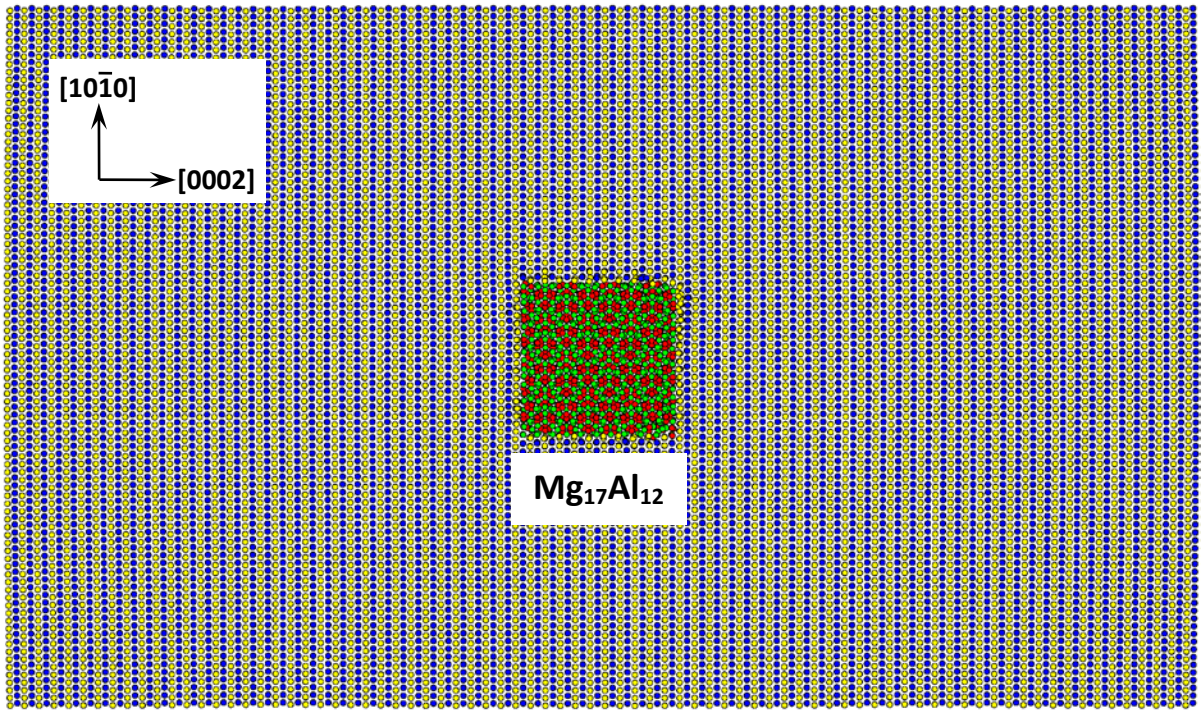
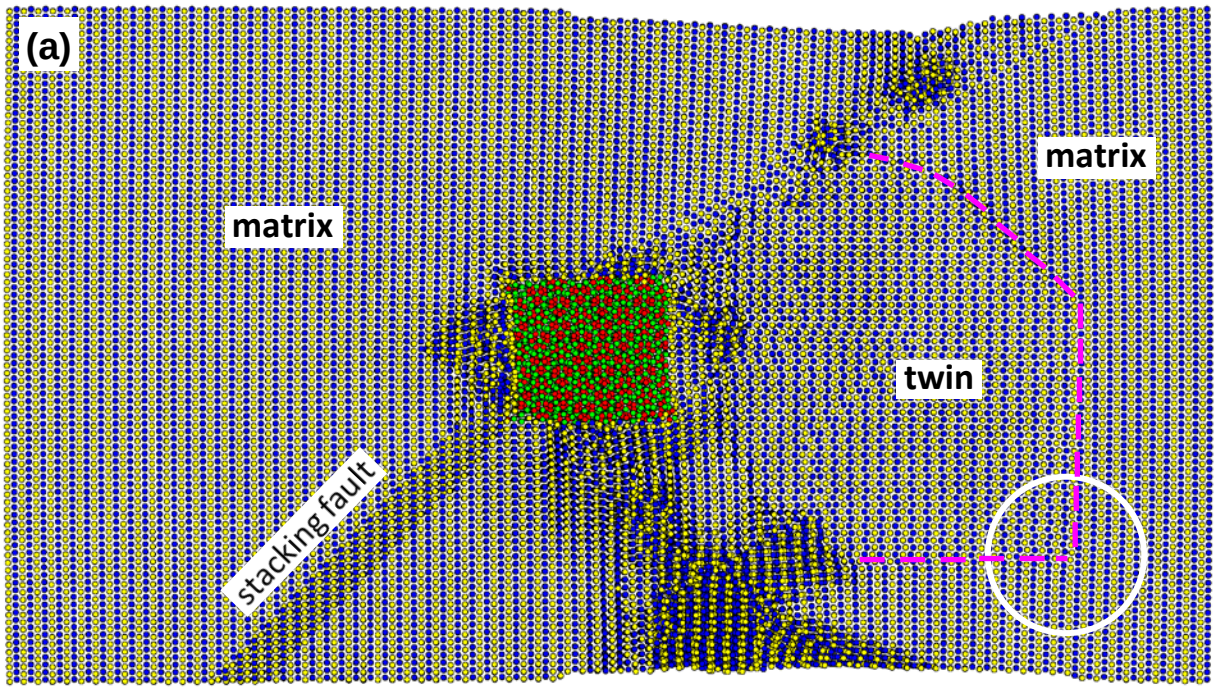
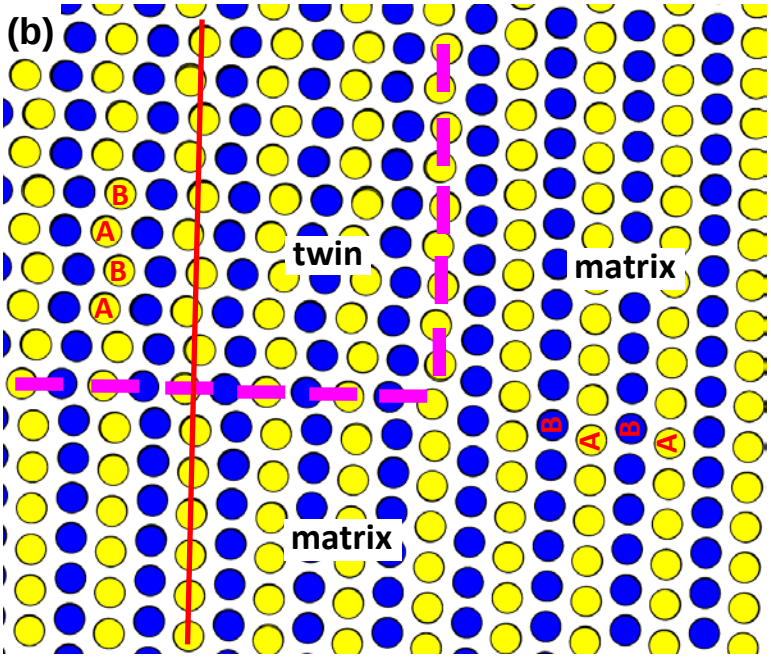


Figure 1. Cross-sectional view of the initial configuration of a Mg single crystal with a β-$Mg_{17}Al_{12}$ precipitate. Only a thin slice (~ 1.5 nm thick) in the middle of through thickness is shown. The basal planes of the matrix are perpendicular to the figure plane, and are colored in yellow and blue to show the *ABABAB*… stacking from left to right. The matrix and the precipitate satisfy the Burgers orientation relationship: $(0001)_M \parallel (011)_P$, and $[2\bar{1}\bar{1}0]_M \parallel [1\bar{1}1]_P$. The system contains over one million atoms. A tensile strain was applied on the left and the right end of the box along the [0002] direction.


(a)
matrix
matrix
twin
stacking fault


(b)
B
A
B
A
twin
matrix
matrix

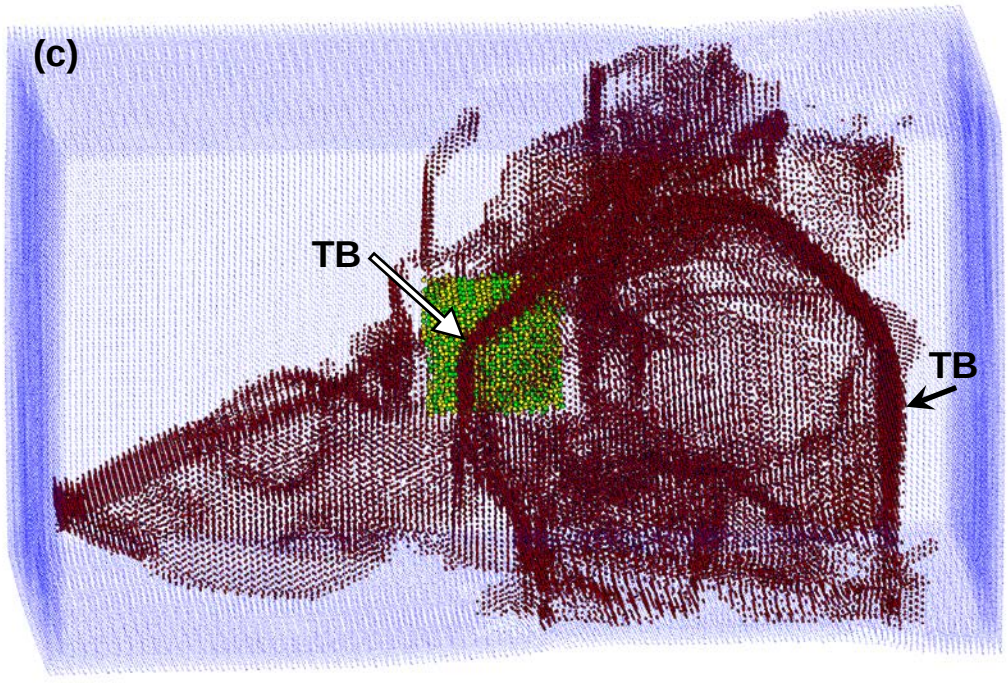


Figure 2. (a) A $\{10\bar{1}2\}$ twin nucleated near the pyramidal dislocations. The twin boundary (TB) is delineated by the dashed pink line. The TB hugely deviates from the $\{10\bar{1}2\}$ twinning plane. (b) The circled area in (a) that comprises both the matrix and the twin was magnified. In the twin (bounded by the dashed line), the stacking of the basal planes is marked with capital letters ABAB… from bottom to top, distinctive from the stacking of the basal planes of the matrix (also marked *with ABAB*… but from left to right). The change in the stacking sequence indicates that twinning reoriented the matrix lattice by about 90º and the $\{10\bar{1}2\}$ twinning indeed took place. After twinning, the initially flat basal planes convert to the corrugated prism planes of the twin, but the atoms remain nearly in the same vertical direction. A vertical straight line demonstrates that zero shear strain was produced by the $\{10\bar{1}2\}$ twinning. (c) 3-D view of the TB. The TB is extremely incoherent. Part of the TB is passing over the precipitate, as indicated by the block arrow.

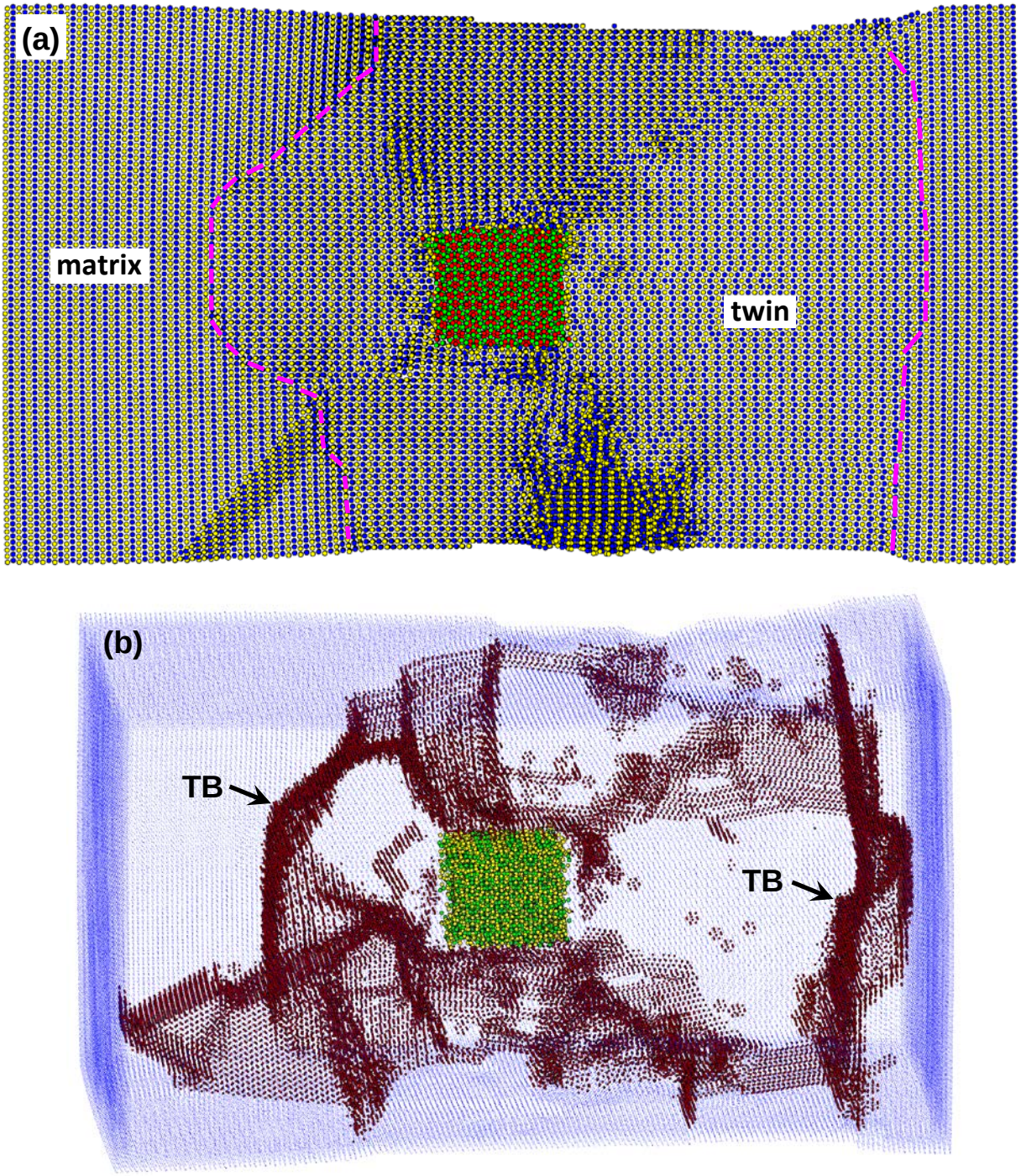


Figure 3. (a) The precipitate is entirely engulfed by the twin without being sheared. The TBs are extremely incoherent. (b) 3-D view. The twinned region expands, digesting the defects generated in the matrix during deformation.